*-- Here we show how to define the crystal field for a d-shell in **D4h symmetry***
-- with 10Dq, Δt2g and Δeg as parameters instead of 10Dq, Dt and Ds.
--The text after "--" is considered by Quanty as a comment.

```
  tenDq    =  1.60
  Dt2g  = 0.1
  Deg   =  0.5
  Ea1g    =  0.6* tenDq + 0.5*Deg              -- energy of the orbital x2-y2
  Eb1g    =  0.6* tenDq - 0.5*Deg              -- energy of the orbital z2
  Eb2g    = -0.4* tenDq + (2.0/3.0)*Dt2g       --  energy of the orbital xy
  Eeg     = -0.4* tenDq - (1.0/3.0)*Dt2g       --  energy of the orbitals xz, yz
Akm = {{0, 0, (1/5)*(Ea1g + Eb1g + Eb2g + (2)*(Eeg))} ,
      {2, 0, Ea1g + (-1)*(Eb1g) + (-1)*(Eb2g) + Eeg} ,
      {4, 0, (3/10)*((6)*(Ea1g) + Eb1g + Eb2g + (-8)*(Eeg))} ,
      {4,-4, (3/2)*((sqrt(7/10))*(Eb1g + (-1)*(Eb2g)))} ,
      {4, 4, (3/2)*((sqrt(7/10))*(Eb1g + (-1)*(Eb2g)))} }
OppCF = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
```

*-- Here we show how to define the crystal field for a d-shell in **D3d symmetry***
-- with 10Dq, and ⊿t2g as parameters instead of 10Dq, Dtau and Dsigma.
-- Here we considered, for example, the setting B (C3//001, C2//100 C4//0t-1).
-- (see next page for other settings)
-- Emix is a mixing term between the Eegpi and Eegsigma orbitals

```
tenDq   = 1.0

Dt2g    = 0.1

Ea1g    = -0.4*tenDq - (2.0/3.0)*Dt2g

Eegpi   = -0.4*tenDq + (1.0/3.0)*Dt2g

Eegsigma = 0.6*tenDq

Emix   = 0

Akm = PotentialExpandedOnClm("D3dB",2,{Ea1g,Eegpi,Eegsigma,Emix})

OppD3dB = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
```

-- The Hybridization for a d-shell in D3d symmetry should be defined in the
-- same settings as the crystal field (D3dB in the present example)

```
Va1g    = 1.1

Vegpi   = 1.1

Vegsigma = 2.2

Vmix   = 0

HYAkm = PotentialExpandedOnClm("D3dB",2,{Va1g,Vegpi,Vegsigma,Vmix})

OppHY = NewOperator("CF", NF, IndexUp_3d,IndexDn_3d,
IndexUp_Ld,IndexDn_Ld,HYAkm) + NewOperator("CF", NF, IndexUp_Ld,IndexDn_Ld,
IndexUp_3d,IndexDn_3d,HYAkm)
```

-- The ligand crystal field in D3d symmetry should be defined in the
-- same settings as the crystal field (D3dB in the present example)
-- even if you fix Dt2gLd = 0.0 to make life easier.

```
tenDqLd  = 1.0

Dt2gLd   = 0.0

Ea1g    = -0.4*tenDq - (2.0/3.0)*Dt2g

Eegpi   = -0.4*tenDq + (1.0/3.0)*Dt2g

Eegsigma = 0.6*tenDq

EmixLd   = 0

LCFAkm = PotentialExpandedOnClm("D3dB",2,{Ea1g,Eegpi,Eegsigma,EmixLd})

OppLCF = NewOperator("CF", NF, IndexUp_Ld, IndexDn_Ld, LCFAkm)
```

Settings in D3d symmetry

--When dealing with linear dichroism in D3d symmetry one has to be careful that the XAS
--will be different not only whether the exchange field (and the spin) is parallel or
--perpendicular to the polarization. The XMLD will depend also on the definition of the crystal
--field, i.e. whether the C2 axis is parallel to the (100), the (010) or the (1-10) axis.
--Five possible definitions (settings) of the D3d crystal field are implemented in Quanty:
--Setting A (C3//001, C2//1-10 C4//111)
--Setting B (C3//001, C2//100 C4//0t-1)
--Setting C (C3//001, C2//100 C4//0t1)
--Setting D (C3//001, C2//010 C4//t0-1)
--Setting E (C3//001, C2//010 C4//t01)
--Here below I show the five possible definitions of the D3d crystal field in an input file for quanty.

```
tenDq    = 1.0

Dt2g     = 0.1

Ea1g     = -0.4*tenDq - (2.0/3.0)*Dt2g

Eegpi    = -0.4*tenDq + (1.0/3.0)*Dt2g

Eegsigma = 0.6*tenDq

Eegmix   = 0

--Setting A (C3//001, C2//1-10 C4//111)

Akm = PotentialExpandedOnClm("D3dA",2,{Ea1g,Eegpi,Eegsigma,Eegmix})

OppD3dA = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)

--Setting B (C3//001, C2//100 C4//0t-1)

Akm = PotentialExpandedOnClm("D3dB",2,{Ea1g,Eegpi,Eegsigma,Eegmix})

OppD3dB = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)

--Setting C (C3//001, C2//100 C4//0t1)

Akm = PotentialExpandedOnClm("D3dC",2,{Ea1g,Eegpi,Eegsigma,Eegmix})

OppD3dC = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)

--Setting D (C3//001, C2//010 C4//t0-1)

Akm = PotentialExpandedOnClm("D3dD",2,{Ea1g,Eegpi,Eegsigma,Eegmix})

OppD3dD = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)

--Setting E (C3//001, C2//010 C4//t01)

Akm = PotentialExpandedOnClm("D3dE",2,{Ea1g,Eegpi,Eegsigma,Eegmix})

OppD3dE = NewOperator("CF", NF, IndexUp_3d, IndexDn_3d, Akm)
```

--Please add in the Hamiltonians H_i and H_f, the crystal field defined according one of the above deinifitions.